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Theory of vibronic optical spectra of impurity centers with violation of the Condon approximation

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Abstract

Expressions for non-Condon generating functions of absorption and luminescence of optical centers in crystals at zero temperature have been obtained in the adiabatic approximation. A solution to the Schrödinger equation for an electronic subsystem has been considered to the first order of the perturbation theory for a vibronic interaction linear in normal coordinates of the vibrational subsystem. The non-Condon form function of the optical transition has been obtained in the form of a convolution operator acting on the normalized Condon form function. It has been proved that, if the optical transition is forbidden in the Condon approximation due to symmetry, the non-Condon form function does not contain a zero-phonon line and the non-Condon form functions of absorption and luminescence are symmetric. © Pleiades Publishing, Ltd 2010.

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